Computational details: The details of PBE calculations are same as in the paper. Gaussian09 was used for PBE0 [1], TPSS and TPSSh [2] calculations. cc-pVTZ (cc-pVTZ-PP for Au) basis sets were used in Gaussian calculations.

Table 1: Optimized geometries of $X_4Au_2(C_5H_5N)_2$, X = H, F-I and CF_3 with PBE0, TPSS and TPSSh. cc-pVTZ basis sets was used. All bond lengths in pm and all angles in degree.

X	Functional	R(Au-Au)	R(Au-N)	R(Au-X)	∠XAuX	∠XAuN
	PBE0	247.8	215.5	163.8	172.8	93.6
H	TPSS	249.4	216.8	165.0	174.0	93.0
	TPSSh	248.6	216.4	164.5	173.6	93.2
	PBE0	250.0	215.7	193.0	179.0	89.5
F	TPSS	252.2	218.0	195.3	178.9	89.4
	TPSSh	251.1	217.2	194.2	178.9	89.5
	PBE0	252.4	217.2	229.2	175.0	92.5
Cl	TPSS	254.6	219.3	231.6	175.3	92.4
	TPSSh	253.4	218.5	230.6	175.1	92.4
	PBE0	253.0	216.7	243.5	174.0	93.0
Br	TPSS	254.9	218.8	245.9	174.0	93.0
	TPSSh	253.8	218.0	244.8	173.9	93.1
	PBE0	254.0	216.4	263.1	172.9	93.5
I	TPSS	255.7	218.6	265.3	172.8	93.6
	TPSSh	254.7	217.8	264.2	172.7	93.7
	PBE0	251.7	215.0	209.2	177.4	88.7
CF_3	TPSS	253.8	217.7	211.2	177.1	88.5
	TPSSh	252.8	216.8	210.4	177.3	88.7

Table 2: Optimized geometries at the level of PBE/TZ2P/SR-ZORA for $X_4Au_2(NH_3)_2$, X = H, F-I, all bond lengths in pm and all angles in degree. ADF was used for these calculations.

X	R(Au-Au)	R(Au-N)	R(Au-X)	∠XAuX	∠XAuN
H	250.4	220.7	165.5	174.9	93.1
F	253.5	219.5	196.7	177.2	91.4
Cl	255.5	219.5	231.4	179.0	88.6
Br	255.6	219.5	247.6	179.7	89.2
I	256.3	220.0	266.1	178.9	90.8

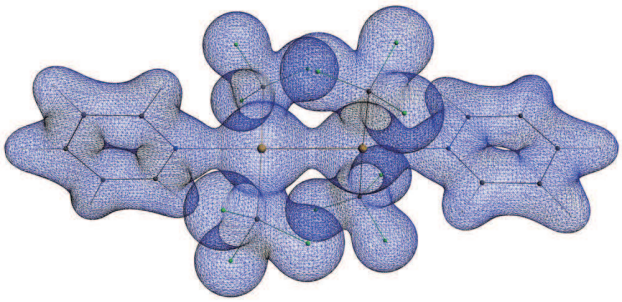

Figure 1: The electron density of $(CF_3)_4Au_2(C_5H_5N)_2$, isosurf. = 0.06 a.u.

References

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